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- Wang, P., R. Nakamura, Y. Kanematsu, Y. Koyama, H. Nagae, T. Nishio, H. Hashimoto and J.-P. Zhang, Low-lying singlet states of carotenoids having 8–13 conjugated double bonds as determined by electronic absorption spectroscopy 410 (2005) 108
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- Winter, B., R. Weber, I.V. Hertel, M. Faubel, L. Vrbka and P. Jungwirth, Effect of bromide on the interfacial structure of aqueous tetrabutylammonium iodide: Photoelectron spectroscopy and molecular dynamics simulations 410 (2005) 222
- Wolszczak, M., M. Steblecka and M. Hilczer, Pulse radiolysis of 9-anthrylmethylammonium cation in aqueous solution 410 (2005) 213
- Woodford, J.N., A DFT investigation of anthocyanidins 410 (2005) 182
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- Xu, Y.Y., X.F. Rui, Y.Y. Fu and H. Zhang, Magnetic properties of α -Fe₂O₃ nanowires 410 (2005) 36
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- Yokomizo, T., J. Higo and M. Nakasako, Patterns and networks of hydrogen-bonds in the hydration structure of human lysozyme 410 (2005) 31
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- Yuan, L.-W., J.-Y. Zhu, Y.-Q. Wang, L. Wang, J.-L. Bai and G.-Z. He, Real-time investigation of the photodissociation dynamics of *p*-chlorotoluene and *p*-dichlorobenzene 410 (2005) 352
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- Zhang, C.-Y., H.-S. Wu and H. Jiao, Structure and stability of endohedral $X@Si_{20}H_{20}$ complexes
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